

A Multiscale Approach to Magnesium Intercalation Batteries: Safer, Lighter, and Longer-Lasting

Completed Technology Project (2017 - 2021)



Project Introduction

Lithium-ion batteries are the gold-standard for electrochemical energy storage; however, the ceiling for their storage potential is constrained by the most fundamental of limits: each lithium-ion only supplies one electron. Safety issues associated with lithium-ion batteries caused by uncontrollable growth of lithium-metal spikes that cause shorts the batteries and can lead to overheating and explosions of the battery as well as the flammability of many lithium-ion battery components are of great concern for the development of space technology and in particular the development of deep-space EVA suits. Broadly, my proposal is to move from lithium and towards magnesium-ion battery technology, by further developing a novel cathode material (one of only a handful in existence), Z-V2O5 which we have previously synthesized in our lab. This material is remarkable, and is capable of reversibly intercalating Mg at room temperature up to a high volumetric capacity. My primary objective is to further develop the nanostructuring of this material and optimize the battery chemistry in order to realize a fully functioning prototype magnesium-ion battery. Furthermore, I will use a variety of characterization and modeling techniques to evaluate this incredible material and inform principles for the intelligent and directed discovery of additional Mg-ion battery cathode materials. To accomplish these goals, I plan to utilize hydrothermal synthesis techniques coupled with structure-directing agents to optimize to optimize the nanostructuring of these materials. I plan to use a diverse palette of topochemical transformations to stabilize the desired empty host structures as well as facile techniques for chemically evaluating magnesium insertion behavior. I will quantify and evaluate the behavior of each phase using DFT+U and Nudged Elastic Band (NEB) calculations to determine expected operating voltages and diffusion barriers. Finally, to evaluate the effects of phase segregation during magnesiation, I will utilize Scanning Transmission X-ray Microscopy (STXM) to map electronic structure domains. Not only does moving from magnesium to lithium theoretically double the amount of charge per unit volume attainable in a cell, but it also allows for the use of Mg metal as an anode, eliminating the need for heavy anode components found in lithium ion batteries (Sn, C) inherently improving the weight of the overall battery. Most importantly, making the switch to magnesium makes batteries inherently safer because magnesium anodes do behave in the same way, forming metal spikes and so avoid the risk of thermal runaway. For these reasons, my proposed research addresses NASA interest in nanostructuring of cathode materials, the development of safer batteries for human life-support systems, and the development of batteries pack more energy into lighter devices (TABS: 10.2.1.4, 3.2.1.1, and 3.2.1.4).

Anticipated Benefits

The proposed research addresses NASA interest in nanostructuring of cathode materials, the development of safer batteries for human life-support systems, and the development of batteries pack more energy into lighter devices.



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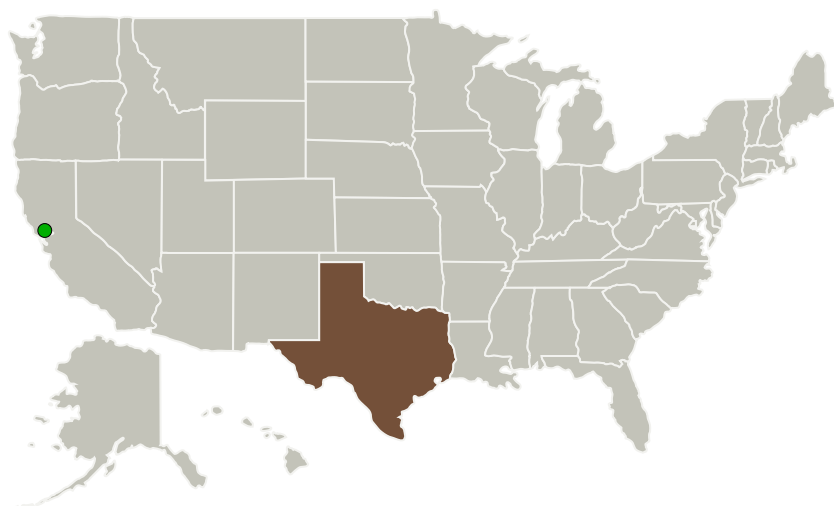
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Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
Texas A & M University-College Station(Texas A&M)	Lead Organization	Academia Hispanic Serving Institutions (HSI)	College Station, Texas
● Ames Research Center(ARC)	Supporting Organization	NASA Center	Moffett Field, California

Primary U.S. Work Locations

Texas

Project Website:

<https://www.nasa.gov/strg#.VQb6T0jJzyE>

Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Lead Organization:

Texas A & M University-College Station (Texas A&M)

Responsible Program:

Space Technology Research Grants

Project Management

Program Director:

Claudia M Meyer

Program Manager:

Hung D Nguyen

Principal Investigator:

Sarbjit Banerjee

Co-Investigator:

Justin L Andrews

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Technology Maturity (TRL)

Start: **2**
Current: **2**
Estimated End: **3**



Technology Areas

Primary:

- TX03 Aerospace Power and Energy Storage
 - └ TX03.2 Energy Storage
 - └ TX03.2.1 Electrochemical: Batteries

Target Destinations

Earth, The Moon, Mars